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A SURVEY OF THE USE OF COMPUTERS IN CHEMICAL RESEARCH AT U.S. UNIVERSITIES

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Robert K. Neuman, Project Administrator
John Robert Jones, Project Coordinator
Harry J. Foxwell, Statistical Analyst
Joanna K. Chin, Project Assistant

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PROCEDURES and SUMMARY

The 1979 Edition of the "Directory of Graduate Research," published by the American Chemical Society, lists 4,471 faculty members at 191 chemistry departments. The names and addresses of all these faculty members were typed onto mailing labels, and a label was affixed to the top portion of each survey questionnaire. On January 7, 1980 the questionnaires were sent out in window envelopes by priority mail.

As each questionnaire came back, an ACS employee made sure that the university name (including branch location) appeared on the lower portion of the questionnaire and then removed the upper portion.

A second mailing of the questionnaire was made on January 29, 1980 to chemists who had not yet responded. By March 14, the cutoff date, 2,567 (57.4%) completed questionnaires had been returned. Between March 24 and April 4 an ACS employee telephoned about 200 persons who had not responded to the mail questionnaire and asked them whether they used computers in their research.

About 68% of those called answered affirmatively. Of those who responded to the mail survey, about 60% had indicated that they used computers, naming specific brands and models. The difference between 60% and 68% is small and may result partly because persons who do little computing might say yes when asked by telephone whether they compute, but respond negatively when asked to write the name and model number of computers they use. Thus, the proportion who use computers in their research was about the same for those who responded to the mail survey as for those who did not, and the results obtained from the mail survey may be safely used to represent all academic chemists.

RESULTS

EXPECTED INCREASE IN COMPUTING

The following table shows that about half of the 1,364 respondents who use computers in their research say they expect to increase use of both small lab computers and centralized computer facilities. Only 7% of the respondents indicated they would not increase their use of either kind of computer.

		Will Increase Use of Small Lab Computer		
		Yes	No	Total
Will Increase Use of Centralized Computer Facilities	Yes	46.0%	8.4%	54.4%
	No	38.4%	7.1%	45.5%
	Total	84.4%	15.5%	100.0%

ARTICLES PUBLISHED

The chemists indicated the number of articles they published in refereed journals from January 1978 through December 1979 ("Published Articles") and how many of those articles reported research that involved using a computer ("Computer Articles").

Chart 1 indicates the extend to which chemists in the various specialties rely on computers for the research they publish.

A majority (55.6%) of theoretical chemists use computers for virtually all the research they publish. On the other hand, most organic chemists (68.2%) and biochemists (55.4%) use computers for less than 5% of the articles they publish.

COMPUTERS

The respondents named the manufacturer and the model of each computer used in their research. An ACS staff member familiar with a wide variety of computers grouped the named computers into four classes according to computing power:

1. "Large" (general-purpose) computers: Typically used in centralized computer facilities. This category includes the IBM 360 and 370, AMDAHL 470, UNIVAC 1100 series, and HONEYWELL 6600.

2. "Mini" (special-purpose) computers: used both by centralized computer centers and by many large laboratories. The many computers in this class include the PDP-11, Data General NOVA, ECLIPSE, and VAX-11.

3. "Micro" computers: Micro-processor-based, desk-top, or small in-lab computers. This group includes the TRS-80, APPLE, WANG, TEXAS INSTRUMENTS, and HEWLETT-PACKARD microcomputers, as well as several listed as "homemade."

4. Unknown type, or non-computers: Hand-held programmable calculators and micro-processor-controlled analytical instruments were frequently listed on the questionnaire. These were not classified as "computers" for this survey and were not tabulated as such. Several unfamiliar computers are also included in this category.

Table 7 contains lists of the manufacturers and models of most computers in each size category. The lists include the number of respondents who use each manufacturer or model.

The following table shows the distribution of computers used by the respondents, according to the categories described above:

Category	Number of Computers	Percent of all Computers
Large	1057	35.0 %
Mini	1171	38.8
Micro	524	17.4
Unknown or Non-computer	265	8.8
Total	3017	100.0 %

QUALITY OF THE GRADUATE FACULTY

Each response was assigned a number representing the estimated quality of the department's graduate faculty. The quality of the graduate faculty was determined using ratings reported in "A Rating of Graduate Programs," Roose and Anderson, American Council on Education, 1970. Roose and Anderson ranked the top 38 departments in order. For this study, the top 19 are category 1, and the next 19 are category 2. Roose and Anderson also placed the next 20 departments in an unranked list, which is category 3 in this study. Roose and Anderson's next 21 departments are category 4. Category 1, which contains 19 top-ranked departments, is divided into two subcategories. Category 1a contains the ten chemistry departments ranked highest according to the Roose-Anderson Rating. Category 1b contains the next nine departments.

Category 5 includes all the remaining 113 departments listed in "The Directory of Graduate Research." Unfortunately, about half the respondents employed by the University of California and several other universities that have campuses in more than one location were not assigned a number representing the quality of graduate faculty. By error, the top portion of their questionnaires were removed without the location of the university branch having been noted.

SPECIALTY AND USE OF NATIONAL COMPUTER SERVICES

Table 1 relates the chemical specialty to whether the chemist uses a computer and to the answers to the use of national computer services. (See Technical Note)

Proportion using computers:

At the extremes, more than 90% of responding theoretical chemists and only 36% of responding organic chemists use computers.

Increase use of computers:

More than 80% of practitioners in every field except theoretical chemistry expect to increase their use of small lab computers, and many also expect to increase their use of large computers. The only field in which fewer than half the specialists expect to increase use of large computers is analytical chemistry.

Use of Computer programs from QCPE and NRCC:

About half of responding organic and theoretical chemists but fewer than a third of respondents in each of the other specialties have used programs from the Quantum Chemistry Program Exchange (QCPE). Except in theoretical chemistry, fewer than 5% of specialists in any field have used programs from the National Resource for Computing in Chemistry (NRCC).

NRCC computer time and customer services:

In every field other than theoretical very few respondents have either obtained grants of computer time from the NRCC or used the NRCC's customer services.

COMPUTER SIZE AND QUESTIONS ABOUT HOW COMPUTERS ARE USED

Chemists use large computers mostly for number crunching, gain access to large computers mostly by batch processing, and generally finance the use of them with university funds. In comparison with the way large computers are used, small computers are much more likely to be used to acquire data and control experiments, to be used with a teletype terminal, and to be paid for by outside grants. (Table 2)

QUALITY OF GRADUATE FACULTY AND USE OF NATIONAL COMPUTER SERVICES

The Roose-Anderson Rating of the quality of chemistry departments' graduate faculty shows that the higher the ranking of the faculty the more likely are faculty members to use computers. But the Roose-Anderson Rating shows no particular relationship to whether a chemist uses QCPE or NRCC services. (Table 3)

NUMBER OF ARTICLES INVOLVING COMPUTING AND USE OF NATIONAL COMPUTER SERVICES

Whether a chemist publishes research that relies on a computer bears little relation to the answers to questions I through L--except that those who publish many articles about work that depend on computers are more likely to use the various services available from the NRCC. (Table 4)

SPECIALTY AND COMPUTER SIZE

Among chemists who use computers, chemical specialty is related to computer size. Nearly half of responding biochemists and analytical chemists do not use any large computer. In contrast less than one-fourth of theoretical chemists who use computers do all their computing on small machines. (Table 5)

SIZE OF COMPUTERS AND USE OF NATIONAL COMPUTER SERVICES

Researchers who already use mini- or micro-computers are more likely to expect to increase their use of small lab computers than are researchers who now use only large computers. Likewise, researchers who already use large computers are more likely to expect to increase their use of large centralized facilities than are researchers who now use only small computers. Among those who use both mini- and micro-computers, more expect to increase use of small lab computers than large computers. Overall, it appears that the use of small computers will grow more rapidly than the use of central computer facilities. (Table 6)

APPENDIX A

This appendix shows further detail relating the quality of graduate faculty to the use of national computer services and to predictions about computer use. Category 1, which contains the 19 top-ranked departments, is divided into two subcategories. Category 1a contains the ten chemistry departments ranked highest according to the Roose-Anderson rating. Category 1b contains the next nine departments.

The two subcategories contrast in their predictions about increasing use of small lab computers and of central computer facilities. Members of the top ten departments are more likely to expect to increase their use of small lab computers, but they are less likely to expect to increase their use of central computing facilities.

APPENDIX B

Some computers (such as the Apple II) have characteristics that definitely make them microcomputers. But because "computing power" increases by gradations and is not precisely measurable, the distinction between microcomputers and minicomputers cannot be clearcut. A similar ambiguity blurs the distinction between minicomputers and large computers. Therefore, if a different person were to assign the various computers to the size categories, a few of the computers might move into the next lower or higher class. Such reclassifications, however, would have little effect on the results presented in this report.

Table 7 contains lists of the manufacturers and models of most computers in each size category. The lists include the number of respondents who use each manufacturer or model.

QUALITY OF THE GRADUATE FACULTY

Category 1

Category 1a

Harvard
California Tech.
California, Berkeley
Stanford
MIT
Illinois
California, Los Angeles
Chicago
Columbia
Cornell

Category 1b

Wisconsin
Yale
Princeton
Northwestern
Iowa State (Ames)
Purdue
California, San Diego
Ohio State
Texas

Category 2

Indiana
Michigan
Minnesota
Rockefeller
Florida State
Johns Hopkins
Michigan State
Penn State
Rice
Washington (Seattle)
Brandeis
Carnegie-Mellon
Case Western Reserve
Colorado
Oregon
Brown
Florida
Notre Dame
Rochester

Category 3

Arizona
Brooklyn Polytech.
Buffalo
California, Davis
California, Riverside
Duke
Georgia
Iowa (Iowa City)
Kansas
Louisiana State
Massachusetts
North Carolina
Oregon State
Pennsylvania
Pittsburgh
Southern California
Utah
Vanderbilt
Washington (St. Louis)
Wayne State

Category 4

Arizona State
Cincinnati
Delaware
Emory
Georgia Tech.
Houston
Illinois Inst. of Tech.
Kansas State
Maryland
NYU
Nebraska
New Hampshire
Rensselaer
Rutgers
Syracuse
Tennessee
Texas A&M
Tulane
Virginia
Virginia Polytech
Washington State

Chart 1

COMPUTER ARTICLES AS A PERCENT OF PUBLISHED ARTICLES

by Specialty

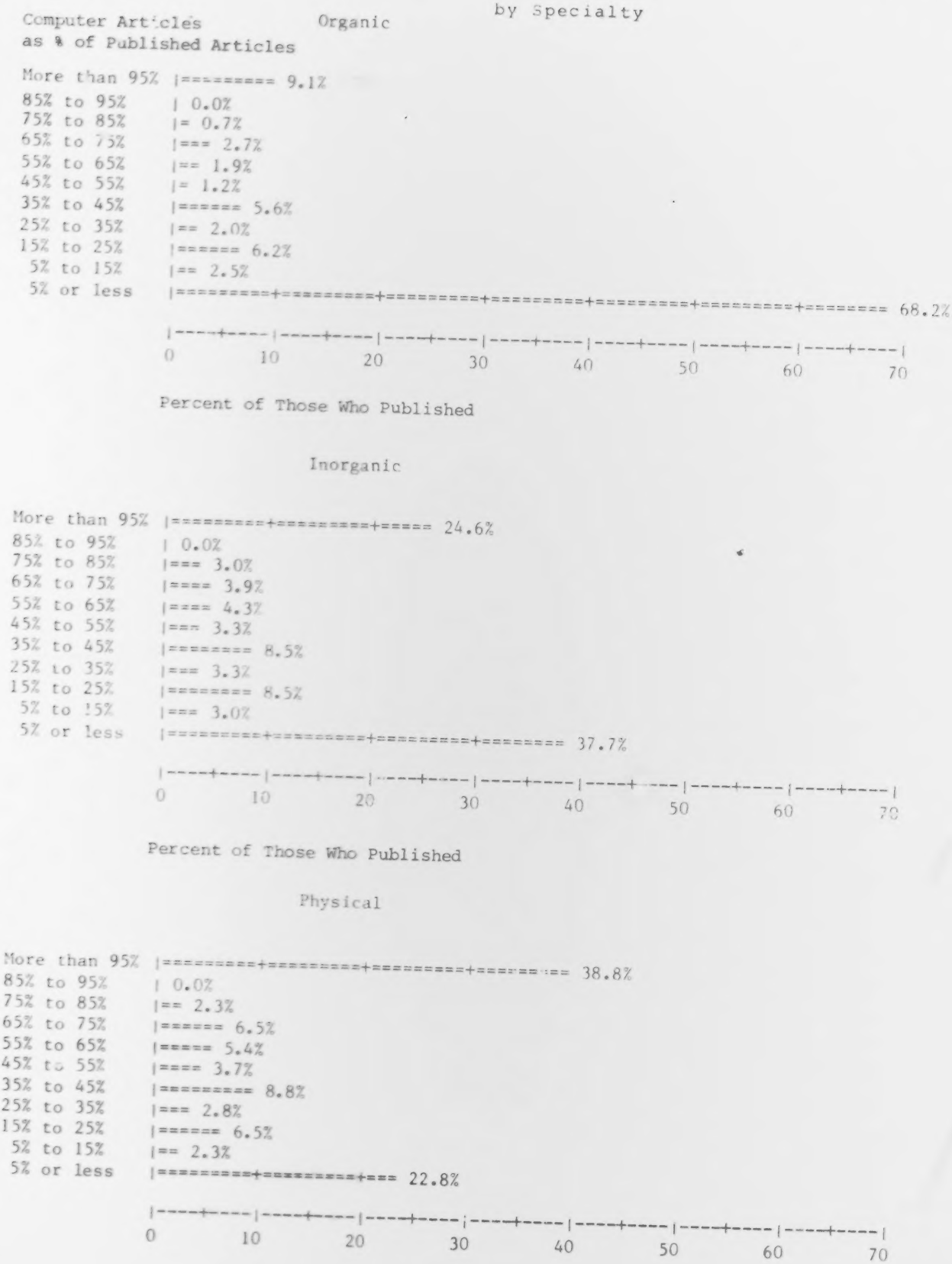
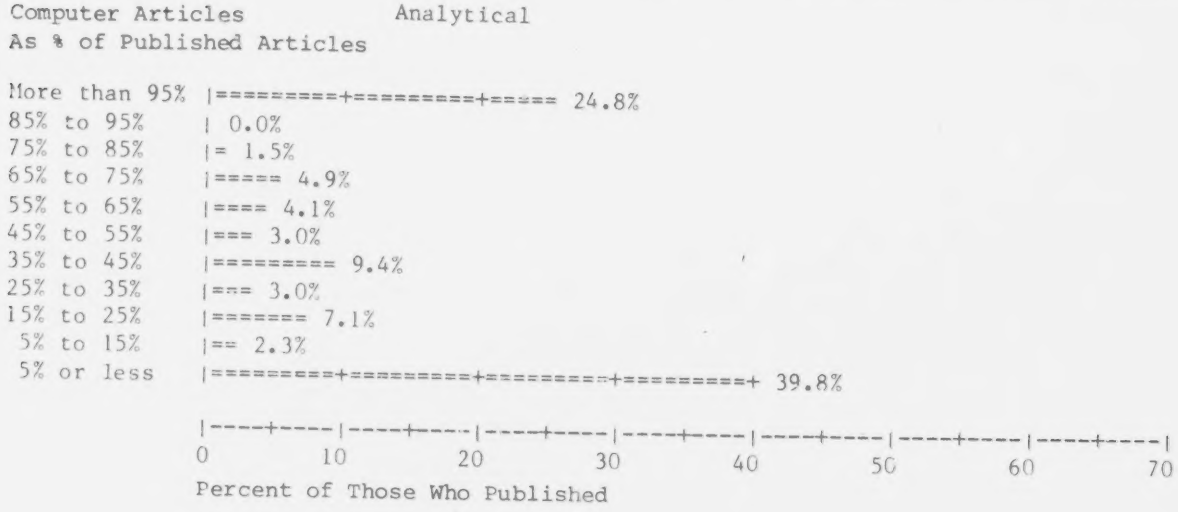
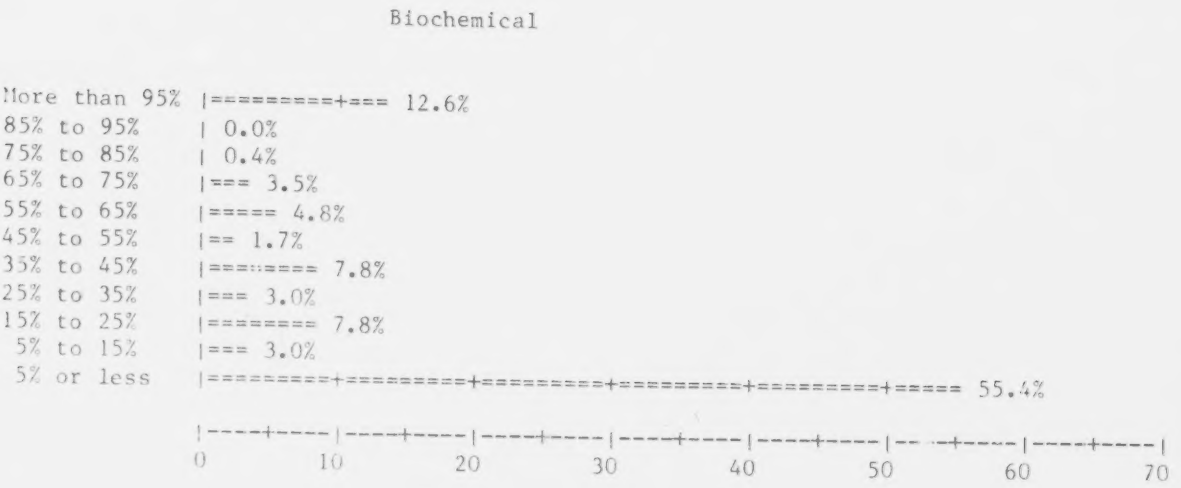

Computer Articles as % of Published Articles
Organic
More than 95% 9.1%
85% to 95% 0.0%
75% to 85% 0.7%
65% to 75% 2.7%
55% to 65% 1.9%
45% to 55% 1.2%
35% to 45% 5.6%
25% to 35% 2.0%
15% to 25% 6.2%
5% to 15% 2.5%
5% or less 68.2%
0 10 20 30 40 50 60 70
Percent of Those Who Published
Inorganic
More than 95% 24.6%
85% to 95% 0.0%
75% to 85% 3.0%
65% to 75% 3.9%
55% to 65% 4.3%
45% to 55% 3.3%
35% to 45% 8.5%
25% to 35% 3.3%
15% to 25% 8.5%
5% to 15% 3.0%
5% or less 37.7%
0 10 20 30 40 50 60 70
Percent of Those Who Published
Physical
More than 95% 38.8%
85% to 95% 0.0%
75% to 85% 2.3%
65% to 75% 6.5%
55% to 65% 5.4%
45% to 55% 3.7%
35% to 45% 8.8%
25% to 35% 2.8%
15% to 25% 6.5%
5% to 15% 2.3%
5% or less 22.8%
0 10 20 30 40 50 60 70
Percent of Those Who Published

Chart 1 COMPUTER ARTICLES AS A PERCENT OF PUBLISHED ARTICLES (continued)





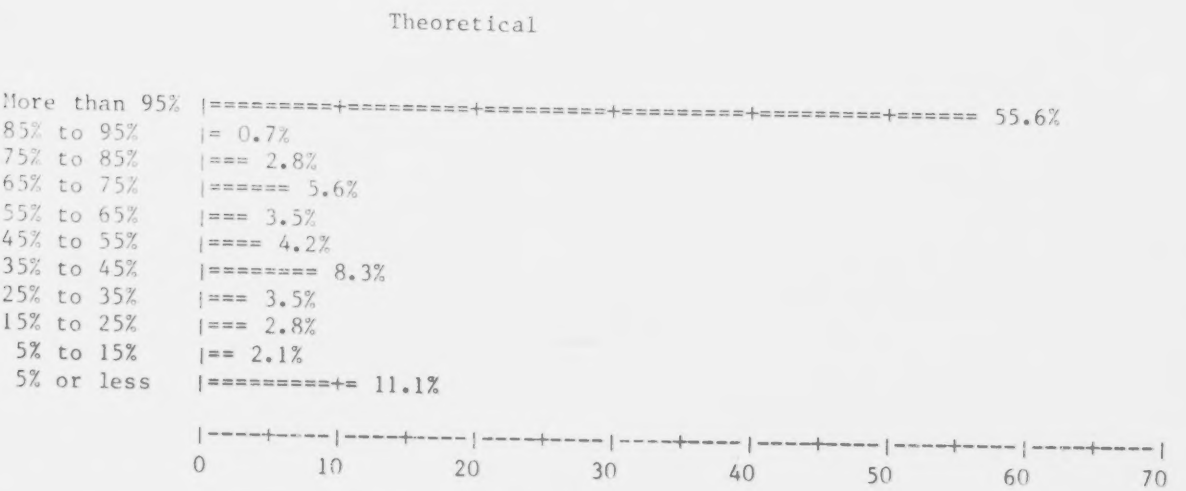


Table 1

Use of National Computer Services and Computer Use Predictions by chemical Specialty

SPECIALTY	Respondents Who Compute (as a per cent of all respondents)	Percent of Those Who Compute: INCREASE SMALL LAB COMPUTER yes	INCREASE CENTRAL FACILITY yes	USED QCPE yes	USED NRCC yes	RECEIVED NRCC GRANT yes	USED NRCC SERVICE yes
Organic	35.7%	82.8%	54.3%	51.2%	3.7%	2.1%	2.1%
	(32.2%-39.4%)	(77.4%-87.1%)	(47.7%-60.7%)	(45.0%-57.4%)	(1.9%-6.8%)	(0.9%-4.7%)	(0.9%-4.8%)
	689	232	221	246	246	243	238
Inorganic	63.9	83.3	56.9	28.6	4.7	1.7	0.9
	(58.9%-68.7%)	(77.9%-87.7%)	(50.2%-63.3%)	(23.2%-34.7%)	(2.6%-8.2%)	(0.7%-4.3%)	(0.2%-3.1%)
	366	222	218	234	234	234	228
Physical	81.4	86.5	55.5	29.4	3.3	2.3	2.1
	(78.3%-84.1%)	(83.3%-89.2%)	(51.2%-59.8%)	(25.7%-33.4%)	(2.1%-5.2%)	(1.3%-3.9%)	(1.2%-3.7%)
	661	526	508	538	538	532	528
Analytical	69.1	92.6	44.3	10.2	2.9	0.5	0.5
	(63.7%-74.1%)	(88.2%-95.9%)	(37.4%-51.5%)	(6.8%-15.1%)	(1.3%-6.2%)	(0.1%-2.7%)	(0.1%-2.7%)
	298	204	185	206	206	205	204
Biochemistry	49.6	91.2	49.6	16.4	3.9	0.0	1.6
	(43.6%-55.7%)	(84.9%-95.0%)	(40.8%-58.4%)	(11.0%-23.8%)	(1.7%-8.8%)	(0.0%-3.0%)	(0.4%-5.7%)
	258	125	121	128	128	126	124
Theoretical	92.8	61.7	70.4	54.2	14.1	15.6	9.1
	(87.6%-96.0%)	(53.1%-69.7%)	(62.2%-77.4%)	(46.0%-62.2%)	(9.3%-20.8%)	(10.5%-22.5%)	(5.3%-15.2%)
	153	128	135	142	142	141	132
Other	26.1	81.1	52.9	24.3	10.8	0.0	0.0
	(19.5%-33.9%)	(65.8%-90.5%)	(36.7%-68.6%)	(13.4%-40.1%)	(4.3%-24.7%)	(0.0%-9.4%)	(0.0%-9.9%)
	142	37	34	37	37	37	
Total	59.6%	84.4%	54.9%	31.3%	4.8%	2.9%	2.2%
	(57.7%-61.2%)	(82.5%-86.2%)	(52.3%-57.5%)	(29.0%-33.7%)	(3.8%-6.0%)	(2.2%-3.9%)	(1.6%-3.1%)
	2567	1474	1422	1531	1531	1518	1489

The three rows in each cell are: 1) the sample proportion, 2) the 95% confidence interval and, 3) the number of chemists who responded to the question. See Technical Note for explanation.

Table 2

Size of Computer and Computer Uses

	MICRO COMPUTERS	MID-SIZE COMPUTERS	LARGE COMPUTERS
USAGE:			
Number crunching	36.5%(32.4%-40.7%)*	47.6%(44.7%-50.4%)	87.3%(85.2%-89.2%)
Data acquisition and experimental control	54.1 (49.7%-58.2%)	43.3 (40.5%-46.2%)	4.9 (3.8%-6.4%)
Other use	9.3 (7.2%-12.2%)	9.1 (7.6%-10.9%)	7.8 (6.3%-9.5%)
	100.0%	100.0%	100.0%
ACCESS:			
Batch processing	17.4%(14.4%-20.8%)	15.4%(13.4%-17.6%)	53.9%(50.9%-56.9%)
Remote entry	6.2 (4.4%-8.5%)	9.1 (7.6%-10.9%)	20.6 (18.2%-23.1%)
Teletype terminal	57.1 (52.8%-61.2%)	65.6 (62.8%-68.3%)	23.6 (21.1%-26.2%)
Other access	19.3 (16.1%-22.9%)	9.9 (8.3%-11.8%)	1.9 (1.2%-2.9%)
	100.0%	100.0%	100.0%
FUNDING;			
Outside grants	40.0%(36.0%-44.3%)	42.7%(40.0%-45.6%)	23.1%(20.6%-25.7%)
Within university	46.5 (42.3%-50.9%)	49.5 (46.7%-52.3%)	73.9 (71.2%-76.5%)
Other arrangements	13.5 (10.9%-16.8%)	7.8 (6.4%-9.5%)	3.0 (2.2%-4.2%)
	100.0%	100.0%	100.0%

* the 95% confidence interval

Table 3

Quality of Graduate Faculty, and Computer Use Prediction and Use of National Computer Services

Quality of Graduate Faculty	Respondents Who Compute (as a per cent of all respondents)	Percent of Those Who Compute			
		INCREASE SMALL LAB COMPUTER yes	INCREASE CENTRAL FACILITY yes	USED QCPE yes	USED NRCC yes
1	71.9% (66.8%-76.5%) 331	84.7% (79.5%-88.8%) 229	45.9% (39.5%-52.5%) 222	27.3% (22.0%-33.3%) 238	7.6% (4.8%-11.6%) 238
2	66.1 (60.8%-71.0%) 330	87.1 (81.9%-91.0%) 209	49.7 (42.9%-56.6%) 199	31.9 (25.8%-38.1%) 218	4.6 (2.5%-8.2%) 218
3	62.1 (56.4%-66.4%) 335	80.7 (74.7%-85.5%) 202	57.4 (50.3%-64.3%) 188	33.7 (27.6%-40.3%) 208	3.4 (1.6%-6.8%) 208
4	61.5 (56.4%-66.4%) 356	82.5 (76.9%-87.1%) 212	54.2 (47.3%-60.9%) 203	28.8 (23.2%-35.1%) 219	6.4 (3.9%-10.4%) 219
5	53.4 (50.4%-56.5%) 1022	85.6 (82.4%-88.4%) 522	60.7 (56.5%-64.9%) 512	34.4 (30.6%-38.5%) 546	3.7 (2.4%-5.6%) 546
Unknown	52.8 (45.8%-59.8%) 193	83.0 (74.5%-89.1%) 100	52.0 (42.3%-61.7%) 98	23.5 (16.4%-32.6%) 102	3.9 (1.5%-9.7%) 102
Total	59.6 (57.7%-61.5%) 2567	84.4% (82.5%-86.1%) 1474	54.9% (52.3%-57.5%) 1422	31.3% (29.0%-33.7%) 1531	4.8% (3.8%-6.0%) 1531

The three rows in each cell are: 1) the sample proportion, 2) the 95% confidence interval and, 3) the number of chemists who responded to the question. See Technical Note for explanation.

Table 3a

Quality of Graduate Faculty, and Computer Use Prediction and Use of National Computer Services

Quality of Graduate Faculty	Respondents Who Compute (as a percent of all respondents)	Percent of Those Who Compute			
		Increase Small Lab Computer Yes	Increase Central Facility Yes	Used QCPE Yes	Used NRCC Yes
1a	71.0% (63.9%-77.0%) 182	88.1% (81.3%-92.7%) 126	37.5% (29.4%-46.4%) 120	26.9% (20.0%-35.1%) 130	7.7% (9.2%-13.6%) 130
1b	72.0% (64.1%-78.3%) 152	80.0% (71.4%-86.5%) 105	55.3% (45.7%-64.6%) 103	29.4% (21.6%-38.5%) 109	7.3% (3.8%-13.8%) 109

The three rows in each cell are: 1) the sample proportion, 2) the 95% confidence interval and, 3) the number of chemists who responded to the question. See Technical Note for explanation.

Table 4

Published Research Involving Computing and Use of National Computer Services

COMPUTER ARTICLES	Respondents Who Compute (as a per cent of all respondents)	Percent of Those Who Compute					
		INCREASE SMALL LAB COMPUTER yes	INCREASE CENTRAL FACILITY yes	USED QCPE yes	USED NRCC yes	RECEIVED NRCC GRANT yes	USED NRCC SERVICES yes
0	25.7%	79.0%	58.2%	26.3%	1.5%	1.3%	0.9%
	(23.4%-28.2%)	(74.1%-83.1%)	(52.5%-63.7%)	(21.8%-31.3%)	(0.7%-3.5%)	(0.5%-3.2%)	(0.3%-2.7%)
	1273	309	299	327	327	320	319
1	80.5	80.1	57.0	24.8	3.8	0.5	1.0
	(75.2%-84.8%)	(74.0%-85.1%)	(49.9%-63.8%)	(19.4%-31.0%)	(1.9%-7.3%)	(0.9%-2.7%)	(0.3%-3.5%)
	261	196	193	210	210	207	204
2-4	94.3	86.2	54.1	32.0	5.1	1.0	1.6
	(92.0%-96.0%)	(82.9%-88.9%)	(49.6%-58.5%)	(28.1%-36.2%)	(3.5%-7.3%)	(0.4%-2.3%)	(0.8%-3.1%)
	543	499	479	512	512	509	500
5-10	98.1	87.7	54.0	35.9	5.3	5.0	3.2
	(96.1%-99.1%)	(83.9%-90.8%)	(48.7%-59.3%)	(31.1%-41.0%)	(3.4%-8.1%)	(3.2%-7.8%)	(1.8%-5.6%)
	366	350	335	359	359	359	348
11 or more	99.2	88.3	49.1	39.0	12.2	13.0	7.6
	(95.6%-99.9%)	(81.4%-92.9%)	(40.2%-58.1%)	(30.9%-47.9%)	(7.5%-19.2%)	(4.5%-14.3%)	(4.1%-13.3%)
	124	120	116	123	123	123	118
Total	59.6	84.4%	54.9%	31.3%	4.8%	2.9%	2.2%
	(57.7%-61.5%)	(82.5%-86.2%)	(52.3%-57.5%)	(29.0%-33.7%)	(3.8%-6.0%)	(2.2%-3.9%)	(1.6%-3.1%)
	2567	1474	1422	1531	1531	1518	1489

The three rows in each cell are: 1) the sample proportion, 2) the 95% confidence interval and, 3) the number of chemists who responded to the question. See Technical Note for explanation.

Table 5

Specialty and Computer Size

SPECIALTY	LARGE ONLY	SMALL AND LARGE	SMALL ONLY	TOTAL
Organic	35.7 (29.7%-42.2%) 80	29.9 (24.3%-36.2%) 67	34.4 (28.5%-40.8%) 77	100.0
Inorganic	26.5 (21.2%-32.7%) 60	46.9 (40.5%-53.4%) 106	26.5 (21.2%-32.7%) 60	100.0
Physical	21.7 (18.3%-25.4%) 112	43.1 (38.9%-47.4%) 223	35.2 (31.2%-39.4%) 182	100.0
Analytical	14.8 (10.5%-20.4%) 29	36.2 (29.8%-43.2%) 71	49.0 (42.1%-55.9%) 96	100.0
Biochemistry	20.2 (13.9%-28.3%) 24	31.1 (23.5%-39.9%) 37	48.7 (39.9%-57.6%) 58	100.0
Theoretical	46.4 (38.4%-54.7%) 65	30.7 (23.7%-38.8%) 43	22.9 (16.7%-30.5%) 32	100.0

The three rows in each cell are: 1) the sample proportion, 2) the 95% confidence interval and, 3) the number of chemists who responded to the question. See Technical Note for explanation.

Table 6

Computer Size, and Computer Use Predictions and Use of National Computer Services

COMPUTER SIZE	Percent of Those Who Compute					
	INCREASE SMALL LAB COMPUTER yes	INCREASE CENTRAL FACILITY yes	USED QCPE yes	USED NRCC yes	RECEIVED NRCC GRANT yes	USED NRCC SERVICES yes
Large	71.8%	65.1%	37.9%	6.5%	4.5%	2.7%
	(66.9%-76.2%)	(60.4%-69.8%)	(33.1%-42.8%)	(4.5%-9.5%)	(2.8%-7.1%)	(1.5%-5.0%)
	358	361	383	383	377	365
Small and large	90.0	57.9	37.7	5.5	4.3	3.1
	(87.2%-92.2%)	(53.7%-62.0%)	(33.8%-41.8%)	(3.9%-7.72%)	(2.9%-6.3%)	(1.9%-4.9%)
	550	541	562	562	560	551
Small	88.0	44.9	21.9	3.1	0.6	1.2
	(84.3%-90.5%)	(40.4%-49.5%)	(18.5%-25.7%)	(1.9%-5.0%)	(0.2%-1.7%)	(0.6%-2.6%)
	499	461	512	512	510	502
Total	84.4	54.9	31.3	4.8	2.9	2.2
	(82.5%-86.5%)	(52.3%-57.5%)	(29.0%-33.7%)	(3.8%-6.0%)	(2.2%-3.9%)	(1.6%-3.1%)
	1474	1422	1531	1531	1518	1489

The three rows in each cell are: 1) the sample proportion, 2) the 95% confidence interval and, 3) the number of chemists who responded to the question. See Technical Note for explanation.

Table 7

COMPUTERS USED BY RESPONDENTS

Small Microcomputers	Number	Percent
AIM (Rockwell)	10	1.9
ALTAIR	9	1.7
APPLE II	18	3.4
COMMODORE (PET)	28	5.3
CROMEMCO	12	2.3
HEATH	7	1.3
HEWLETT-PACKARD - 3000	26	5.0
- 98XX	31	5.9
- Other	38	7.3
HOMEMADE	12	2.3
IBM (5100)	3	0.6
IMSAI	11	2.1
INTEL	16	3.1
ITEL	27	5.2
KIM	14	2.7
NICOLET	94	17.9
NORTHSTAR	8	1.5
OHIO SCIENTIFIC	7	1.3
RADIO SHACK (TRS-80)	22	4.2
TEKTRONIX	34	6.5
TEXAS INSTRUMENTS - 9XX	35	6.7
WANG	12	2.3
Others	50	9.5
T O T A L :	524	100.0

Table 7 (continued)

COMPUTERS USED BY RESPONDENTS

Small/Large Minicomputers		Number	Percent
CDC		17	1.5
DATA GENERAL	-NOVA	145	12.4
	-ECLIPSE	17	1.5
	-Other	8	0.7
DEC	-PDP-8	163	13.9
	-PDP-10	135	11.5
	-PDP-11	341	29.1
	-VAX-11	62	5.3
	-PDP-20	27	2.3
	-LSI-11	37	3.2
	-PDP-12	14	1.2
	-Other	27	2.3
HARRIS		20	1.7
IBM	-30XX	54	4.6
	-70XX	9	0.8
	-Other	7	2.4
PRIME		28	0.6
RAYTHEON		7	0.6
VARIAN 620		39	3.3
Others		14	1.2
	T O T A L :	1171	100.0*

* Detail may not add to total because of round-off error.

Table 7 (continued)

COMPUTERS USED BY RESPONDENTS

Large Main-Frames	Number	Percent
AMDAHL	86	8.0
BURROUGHS	36	3.4
CDC	309	28.8
HONEYWELL	26	2.4
IBM - 360/X	147	13.7
- 370/X	304	28.4
- Other	23	2.2
UNIVAC 11XX	84	7.8
XEROX	42	3.9
Others	15	1.4
T O T A L :	1072	100.0

TECHNICAL NOTE

Number answering various questions.

Some persons failed to answer one or more questions, and so the number of respondents differs from question to question. For the questions of how many NRCC and QCPE programs the chemist used, however, failure to answer was interpreted to mean "none". Thus, the tables show the number of persons responding to those two questions as the total number who compute (1531). The number of respondents to the other questions is less than 1531, because those questions are subject to non-response.

Sample proportions

The text is worded as though the sample proportions were exactly equal to the population proportions. A more refined procedure involves confidence intervals. A 95% confidence interval appears directly below each proportion presented in the tables. For example, consider the proportion of organic chemists expecting to increase their use of small lab computers. Table 1 shows that 82.8% of the organic chemists responding to the survey do expect to increase their use of small lab computers. Thus, about 82.8% of all organic chemists in the surveyed population expect to increase use of small lab computers.

The 95% confidence interval (77.4% to 87.1%) measures the precision of the estimate. The meaning of the phrase "95% confidence" is that if we draw a large number of samples and construct one confidence interval based on each sample, then 95% of the confidence intervals will contain the population proportion.

American Chemical Society

DEPARTMENT OF PROFESSIONAL
RELATIONS AND MANPOWER STUDIES

1155 SIXTEENTH STREET, N.W.
WASHINGTON, D.C. 20036
Phone (202) 872-4600

January 2, 1980

Dear Chairman:

The American Chemical Society has contracted with the National Science Foundation to obtain information concerning how chemists use computers in their research. This information will, I am sure, be useful to chemistry researchers and university administrators. Because computing technology is changing rapidly, understanding and evaluating this research tool depends on up-to-date information about how chemists do their computing.

A sample copy of a form designed to gather such information is enclosed. The American Chemical Society will mail this form to each regular faculty member of your department during the next week or two.

I hope you will encourage members of your department to complete and return the form promptly. The American Chemical Society will make the results of this project available to you. The findings will be reported only in such a way that no information can be attributed specifically to your institution.

If you have any questions concerning the enclosed form or other aspects of the project, I shall be glad to provide further information.

Sincerely,

Robert K. Neuman, Head

RKN/jc
Enclosure

American Chemical Society

DEPARTMENT OF PROFESSIONAL
RELATIONS AND MANPOWER STUDIES

1155 SIXTEENTH STREET, N.W.
WASHINGTON, D.C. 20036
Phone (202) 872-4600

January 7, 1980

Dear Colleague:

Chemical researchers increasingly rely upon assistance from electronic computers. Yet, little information is available about this rapidly changing aspect of chemical research. The chemical profession needs answers to such questions as

- How do academic chemists use computers?
- What kinds of computers do they use?
- How will their computing change in the future?

The American Chemical Society, under contract to the National Science Foundation, is gathering data that will help answer these and related questions. The results of this project will be made available to you and, I believe, prove informative and useful to your department.

Please complete and return the enclosed form. Your participation in this project is, of course, entirely voluntary; not answering some or all of the questions will in no way adversely affect you or your institution.

To guarantee confidentiality, someone not otherwise associated with this project will remove your name as soon as the American Chemical Society receives your completed form. Results will be reported only in such a way that no specific information can be attributed to your institution.

The American Chemical Society is conducting this project under authority of the National Science Foundation Act of 1950, as amended.

Sincerely

Robert K. Neuman, Head

RKN/jc
Enclosure

American Chemical Society

DEPARTMENT OF PROFESSIONAL
RELATIONS AND MANPOWER STUDIES

1155 SIXTEENTH STREET, N.W.
WASHINGTON, D.C. 20036
Phone (202) 872-4600

January 29, 1980

Dear Colleague:

About three weeks ago I wrote to ask you to provide information for a research project that the American Chemical Society is conducting under contract to the National Science Foundation. Many chemists already have replied. And your reply might be in the mail as I write this. If so, please accept out thanks.

In the event that you have not yet replied, I urge you to complete the enclosed form and join your colleagues who have already supplied information. Our hope is that nearly all academic researchers will participate so that this project can benefit our profession as much as possible.

The results of the project will be made available to you and will, I believe, prove informative and useful to your department.

Please complete and return the enclosed form. Your participation in this project is, of course, entirely voluntary; not answering some or all of the questions will in no way adversely affect you or your institution.

To guarantee confidentiality, someone not otherwise associated with this project will remove your name as soon as the American Chemical Society receives your completed form. Results will be reported only in such a way that no specific information can be attributed to your institution.

The American Chemical Society is conducting this project under authority of the National Science Foundation Act of 1950, as amended.

Sincerely,

Robert K. Neuman, Head

RKN/nb
Enclosure

ACS UTILIZATION STUDY

Computers in Academic Chemical Research

A person not otherwise concerned with this survey will detach the top portion of this questionnaire and note that you have responded so that you will not receive a follow-up questionnaire. No one will use your name in any way except to control for non-response.

Please use the margins or the reverse page for more detailed answers or for any comments you might wish to include.

A. Principal academic employer: _____

B. Number of articles you published in refereed journals during the two years from January, 1978 through December, 1979: _____

How many of these articles report research that involved using a computer? ____

C. Which one chemical specialty is most closely related to your research?

___organic	___physical	___biochemical
___inorganic	___analytical	___theoretical

If your research group does not use a computer, STOP. Please return this questionnaire in the envelope provided.

D. What computers, including minicomputers, does your research group use? Please specify model.

	Manufacturer	Model
(1)	_____	_____
(2)	_____	_____
(3)	_____	_____
(4)	_____	_____

E. During a calendar year approximately how many hours of CPU time does your group use on each computer specified in question D?

(1)	(2)	(3)	(4)
___hrs	___hrs	___hrs	___hrs

F. For each computer approximately how are the hours in question E distributed among various uses?

	(1)	(2)	(3)	(4)
"Number crunching"	___%	___%	___%	___%
Data acquisition and experimental control	___%	___%	___%	___%
Other (Specify)_____	___%	___%	___%	___%
TOTAL	100%	100%	100%	100%

G. For each computer approximately how are the hours in question E distributed among various means of access?

	(1)	(2)	(3)	(4)
Batch processing	___%	___%	___%	___%
Remote job entry	___%	___%	___%	___%
Teletype terminal	___%	___%	___%	___%
Other (Specify)_____	___%	___%	___%	___%
TOTAL	100%	100%	100%	100%

H. For each computer approximately how are the hours in question E financed?

	(1)	(2)	(3)	(4)
Grants from outside university	___%	___%	___%	___%
Sources within university	___%	___%	___%	___%
Other arrangements	___%	___%	___%	___%
TOTAL	100%	100%	100%	100%

I. Do you expect that during the next five years your group will increase its:

computing in the laboratory on small computers? [ ] Yes [ ] No
computing at a centralized facility? [ ] Yes [ ] No

J. How many different programs has your research group used from:

QCPE (The Quantum Chemistry Program Exchange)? ___Programs
NRCC (The National Resource for Computing in Chemistry)? ___Programs
Other (Specify) ___Programs

K. Has your research group received a grant of computer time at NRCC? [ ] Yes [ ] No

L. Has your research group used the customer services of NRCC? [ ] Yes [ ] No

Please return this form to the American Chemical Society
Room 312, 1155 Sixteenth St., NW, Washington, D.C. 20036
Thank you